

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

**Predicted value:** 1.55

**Global applicability domain:** Inside

**Local applicability domain index:** 4.79e-01

**Confidence level:** 3.02e-01

Nearest Neighbors from the Training Set

Image not found

Clofencet

**Measured:** -2.20

**Predicted:** 1.42

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8-Methylcinnolin-4-amine

**Measured:** 1.57

**Predicted:** 5.55e-01